Snowmass'21

Accelerator Frontier Computational Needs

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Computational Frontier Workshop

August 10-11, 2020

Accelerator Frontier @ Snowmass21

- AF1: Beam Physics and Accelerator Education
- AF2: Accelerators for Neutrinos
- AF3: Accelerators for EW/Higgs
- AF4: Multi-TeV Colliders
- AF5: Accelerators for PBC and Rare Processes
- AF6: Advanced Accelerator Concepts
- AF7: Accelerator Technology R&D
  - RF
  - Magnets
  - Targets/Sources

All these activities rely on computation at some point, sometimes requiring massively parallel supercomputing.

SciDAC
Scientific Discovery through Advanced Computing

ECP EXASCALE COMPUTING PROJECT

Computational needs are large and varied

- End product is the particle beam(s) before collisions (or other usage)
- Prediction of final beam needs tracking from inception and through all acceleration and manipulation processes
  - From single particle dynamics to tightly coupled many-particles dynamics.
  - Including RF fields, magnets, pipes, etc and for very long time in rings (many time steps).
- Many types of machines
  - Linacs, rings, recirculators, energy recovery systems, fixed-field accelerators, plasma accelerators, dielectric accelerators, targets, …
- Full physics implies many effects
  - Halos, wakefields, impedance, electron cloud, beam-beam, collisions, secondary emission, spin dynamics, (in)coherent synchrotron radiation, painting, …
  - Design/analysis of accelerator components.
- Design implies ensembles, incl. multi-obj. optimization & Machine Learning

Trend is toward increasing needs for computing

Four grand challenges from DOE HEP GARD Accel. & Beam Physics Workshops

1. **Intensity** - Increase beam intensities by orders of magnitude.
2. **Quality** - Increase beam phase-space density by orders of magnitude, towards quantum degeneracy limit.
3. **Control** - Control the beam distribution down to the level of individual particles.
4. **Prediction** - Develop predictive start-to-end "virtual particle accelerators".

➔ More particles, higher fidelity, more physics, more integration.

➔ Will benefit from (needs for some topics) larger/faster exascale (and post-exascale) supercomputers, especially for design work (i.e., large ensembles) and develop ML models.

Status: many codes

- E.g., conventional accelerator and beam physics codes
  - Mostly single developers; a few frameworks & a few teams.

Beam dynamics codes section from Accelerator Handbook (A. Chao, 2013)

Very dynamic community with many innovations in algorithms pushing the field forward.

But is there some duplication?

Disclaimer: list may be incomplete.

Beam Dynamics Codes:

(Below, PIC refers to codes with particle-in-cell space-charge capability.)

Code	URL or Contact	Description/Comments
ASTRA	tesla.desy.de/~meykopff	3D parallel, general charged particle beams incl. space charge
AT	sourceforge.net/projects/atcollab/	Accelerator Toolbox
BETACOOL	betacool.jinr.ru	Long term beam dynamics: ECOOL, IBS, internal target
Bmad, Tao	www.lns.cornell.edu/~dcs/bmad/	General purpose toolbox library + driver program
COSY INFINITY	www.cosyinfinity.org	Arbitrary-order beam optics code
CSRTrack	www.desy.de/xfel-beam/csrtrack	3D parallel PIC; includes CSR; mainly for e^- dynamics
Elegant/SDDS suite	aps.anl.gov/elegant.html	parallel; track, optimize; errors; wakes; CSR
ESME	www-ap.fnal.gov/ESME	Longitudinal tracking in rings
HOMDYN	Massimo.Ferrario@LNF.INFN.IT	Envelope equations, analytic space charge and wake fields
IMPACT code suite	amac.lbl.gov	3D parallel multi-charge PIC for linacs and rings
LAACG code suite	laacg.lanl.gov	Includes PARMILA, PARMELA, PARMTEQ, TRACE2D/3D
LiTrack	www.slac.stanford.edu/~emma/	Longitudinal linac dynamics; wakes; GUI-based; error studies
LOCO	safranek@slac.stanford.edu	Analysis of optics of storage rings; runs under matlab
LUCRETIA	www.slac.stanford.edu/accel/ilc/codes	Matlab-based toolbox for simulation of single-pass e^- systems
MaryLie	www.physics.umd.edu/dsat	Lie algebraic code for maps, orbits, moments, fitting, analysis
MaryLie/IMPACT	amac.lbl.gov	3D parallel PIC; MaryLie optics + IMPACT space charge
MAD-X	mad.web.cern.ch/mad	General purpose beam optics
MERLIN	www.desy.de/~merlin	C++ class library for charged particle accelerator simulation
OPAL	amas.web.psi.ch	3D parallel PIC; cyclotrons, FFAGs, linacs; particle-matter int.
ORBIT	jzh@ornl.gov	Collective beam dynamics in rings and transport lines
PATH	Alessandra.Lombardi@cern.ch	3D PIC; linacs and transfer lines; matching and error studies
SAD	acc-physics.kek.jp/SAD/sad.html	Design, simulation, online modeling & control
SIMBAD	agsrhichome.bnl.gov/People/luccio	3D parallel PIC; mainly for hadron synchrotrons, storage rings
SIXTRACK	frs.home.cern.ch/frs/	Single particle optics; long term tracking in LHC
STRUCT	www-ap.fnal.gov/users/drozhdin	Long term tracking w/ emphasis on collimators
Synergia	https://compacc.fnal.gov/projects	3d parallel PIC; space charge, nonlinear tracking and wakes
TESLA	lyyang@bnl.gov	Parallel; tracking; analysis; optimization
TRACK	www.phy.anl.gov/atlas/TRACK	3D parallel PIC, mainly for ion or electron linacs
LIBTRACY	libtracy.sourceforge.net/	Library for beam dynamics simulation
TREDI	www.tredi.enea.it	3D parallel PIC; point-to-point Lienard-Wiechert
UAL	code.google.com/p/ual/	Unified Accelerator Libraries
WARP	DPGrote@lbl.gov	3D parallel ES and EM PIC with accelerator models
ZGOUBI	sourceforge.net/projects/zgoubi/	Magnetic optics; spin; sync radiation; in-flight decay

Status: many codes

- E.g., plasma accelerator codes
  - Mostly single developers; a few frameworks & a few teams.

Plasma accelerator codes
From J.-L. Vay, R. Lehe,
RAST 9 (2016)

Very dynamic community with many innovations in algorithms pushing the field forward.

But is there some duplication?

Table 1. List of simulation PIC codes for the modeling of plasma accelerators.

Code	Type	Website/reference	Availability/license
ALaDyn/PICCANTE	EM-PIC 3D	http://aladyn.github.io/piccante	Open/GPLv3+
Architect	EM-PIC RZ	https://github.com/albz/Architect	Open/GPL
Calder	EM-PIC 3D	http://iopscience.iop.org/article/10.1088/0029-5515/43/7/317	Collaborators/Proprietary
Calder-Circ	EM-PIC RZ$^+$	http://dx.doi.org/10.1016/j.jcp.2008.11.017	Upon Request/Proprietary
CHIMERA	EM-PIC RZ+	https://github.com/hightower8083/chimera	Open/GPLv3
ELMIS	EM-PIC 3D	http://www.diva-portal.org/smash/record.jsf?pid=diva2%3A681092&dswid=-8610	Collaborators/Proprietary
EPOCH	EM-PIC 3D	http://www.ccpp.ac.uk/codes.html	Collaborators/GPL
FBPIC	EM-PIC RZ$^+$	https://fbpic.github.io	Open/modified BSD
HiPACE	QS-PIC 3D	http://dx.doi.org/10.1088/0741-3335/56/8/084012	Collaborators/Proprietary
INF&RNO	QS/EM-PIC RZ	http://dx.doi.org/10.1063/1.3520323	Collaborators/Proprietary
LCODE	QS-PIC RZ	http://www.inp.nsk.su/∼lotov/lcode	Open/None
LSP	EM-PIC 3D/RZ	http://www.lspsuite.com/LSP/index.html	Commercial/Proprietary
MAGIC	EM-PIC 3D	http://www.mrcwdc.com/magic/index.html	Commercial/Proprietary
Osiris	EM-PIC 3D/RZ$^+$	http://picksc.idre.ucla.edu/software/software-production-codes/osiris	Collaborators/Proprietary
PHOTON-PLASMA	EM-PIC 3D	https://bitbucket.org/thaugboelle/ppcode	Open/GPLv2
PICADOR	EM-PIC 3D	http://hpc-education.unn.ru/en/research/overview/laser-plasma	Collaborators/Proprietary
PIConGPU	EM-PIC 3D	http://picongpu.hzdr.de	Open/GPLv3+
PICLS	EM-PIC 3D	http://dx.doi.org/10.1016/j.jcp.2008.03.043	Collaborators/Proprietary
PSC	EM-PIC 3D	http://www.sciencedirect.com/science/article/pii/S0021999116301413	Open/GPLv3
QuickPIC	QS-PIC 3D	http://picksc.idre.ucla.edu/software/software-production-codes/quickpic	Collaborators/Proprietary
REMP	EM-PIC 3D	http://dx.doi.org/10.1016/S0010-4655(00)00228-9	Collaborators/Proprietary
Smilei	EM-PIC 2D	http://www.maisondelasimulation.fr/projects/Smilei/html/licence.html	Open/CeCILL
TurboWave	EM-PIC 3D/RZ	http://dx.doi.org/10.1109/27.893300	Collaborators/Proprietary
UPIC-EMMA	EM-PIC 3D	http://picksc.idre.ucla.edu/software/software-production-codes/upic-emma	Collaborators/Proprietary
VLPL	EM/QS-PIC 3D	http://www.tp1.hhu.de/∼pukhov/	Collaborators/Proprietary
VPIC	EM-PIC 3D	http://github.com/losalamos/vpic	Open/BSD clause-3 license
VSim (Vorpal)	EM-PIC 3D	https://txcorp.com/vsim	Commercial/Proprietary
Wake	QS-PIC RZ	http://dx.doi.org/10.1063/1.872134	Collaborators/Proprietary
Warp	EM-PIC 3D/RZ$^+$	http://warp.lbl.gov	Open/modified BSD

EM = electromagnetic; QS = quasistatic; PIC = particle-in-cell; 3D = three-dimensional; RZ = axisymmetric; RZ$^+$ = axisymmetric with azimuthal Fourier decomposition.

Disclaimer: list may be incomplete.

Looking forward

- Modernization (with support from SciDAC, Exascale Computing Project, …):
  - **Multilevel parallelization**, porting to **GPUs**, …
  - **Advanced algorithms** (high-order solvers, adaptive mesh refinement, long time scales, …).
  - Down the road: potential use of **quantum algorithms and computers**.
- Community development:
  - Tools: e.g., **open source** accelerator toolkit library a la Geant4?
  - Organization: **CAMPA, CBB, HEP-CCE**, …
- Standardization of I/Os, :
  - **Lattice description**: e.g., Mad-X lattice syntax (widely used).
  - **Particle & mesh data**: e.g., openPMD (adopted by growing # of codes & projects).
  - **Code input scripts**: e.g., PICMI (nascent).

➔ **Facilitate benchmarking, workflows, ML, common data analysis software, ...**

Calls for increased resources

- Code development, maintenance, sustainability & reliability
  - Development on **new platforms** is **increasingly complex**.
  - Most efficient with teams of **domain specialists** (beam/accelerator/plasma/… physicists) + **software engineers** + **computer scientists** + **applied mathematicians**.
- User support
  - Codes can be **very complex to use** (many input parameters, numerical effects, …).
  - Needs **good documentation** & **human support**.
- Training
  - **Specific training** needed (USPAS, CAS, …).
  - **Cloud computing** (E.g., Sirepo) can be very effective.

➔**Center(s)** funded by new **DOE Accelerator R&D and Production Program?**

➔**Broad community support** will help getting the needed resources.

Many opportunities for interactions with CompF1-7 and cross-cutting computational needs with other frontiers.

Thank you for your attention.